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# A New Positive Definite Geometric Mean of Two Positive Definite Matrices

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ABSTRACT

We introduce and study a new positive definite (in certain singular cases, positive semidefinite) geometric mean of two positive definite (under certain conditions, positive semidefinite) matrices. © *Elsevier Science Inc., 1997*

## 1. INTRODUCTION AND PRELIMINARIES

In 1978, T. Ando [1] showed that it is possible to extend the notion of geometric mean to positive operations on Hilbert space. [By a positive operator we mean a positive semidefinite operator, i.e. an operator $T$ for which $(Tx, x) \geqslant 0$ for all $x$; we write $T \geqslant 0$ in this case.] Ando starts by

* Research supported by grant A130407.

*LINEAR ALGEBRA AND ITS APPLICATIONS* 251:1–20 (1997)

© Elsevier Science Inc., 1997
655 Avenue of the Americas, New York, NY 10010

0024-3795/97/$17.00
SSDI 0024-3795(95)00540-8

considering two positive operators $A$, $B$ on a Hilbert space $\mathscr{H}$ such that $A^{-1}$ exists. Given any positive $X$, define the operator matrix

$$T(X) = \begin{pmatrix} A & X \\ X & B \end{pmatrix}.$$

The operator $G(A, B) = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}$ is maximal among all positive $X$ for which $T(X) \geqslant 0$. It is thus natural to call it the *geometric mean* of $A$ and $B$. Ando proves the identity $G(A, B) = G(B, A)$ and shows that $G(A, B)$ is dominated by the arithmetic mean of $A$ and $B$. If $A$ and $B$ commute, then clearly $G(A, B) = A^{1/2}B^{1/2}$.

In the course of their investigations of a completion problem [3] the authors found another natural function $F$ of two positive operators which possesses some of the important properties of a geometric mean. In the present note we describe the properties of this new notion of geometric mean and confront it with the mean introduced by Ando. In order to do so we examine more closely the properties of the function $G$ and compare them with analogous properties of the mean $F$.

On the other hand, the most outstanding property of $F$ is the fact that its square is similar to the product $AB$; in particular, the eigenvalues of $F$ coincide with the positive square roots of the eigenvalues of $AB$. These two facts explain why we propose to call $G$ the *metric* and $F$ the *spectral* geometric mean of $A$ and $B$.

In the last section we examine more closely the case when one or both of the operators $A$ and $B$ becomes singular.

## 2. THE METRIC GEOMETRIC MEAN

The first theorem will survey characteristic properties of $G$ for the case that both $A$ and $B$ are $n$-by-$n$ positive definite matrices. We limit ourselves to the finite-dimensional case; most of the results remain valid for operators on Hilbert space. Properties 3, 6, and 7 are new; these last two are closely related to Theorem 2.7 in [4].

THEOREM 2.1. *Let $A$, $B$, and $G$ be positive definite matrices of order $n$. Then the following are equivalent*:

1. $A = GB^{-1}G$;
2. $G = B^{1/2}(B^{-1/2}AB^{-1/2})^{1/2}B^{1/2}$;
3. *there exists a unitary matrix $U$ such that*

$$G = A^{1/2}UB^{1/2};$$

4. $\operatorname{rank}\begin{pmatrix} A & G \\ G & B \end{pmatrix} = n$;

5. *for every $x$, there exists a $y$ such that both relations $Ax = Gy$ and $Gx = By$ hold*;

6. $|(Gx, y)| \leqslant (Ax, x)^{1/2}(By, y)^{1/2}$ *for all $x$ and $y$, and for every $x$, equality is attained for some $y \neq 0$*;

7. $2\operatorname{Re}(Gx, y) \leqslant (Ax, x) + (By, y)$ *for all $x$ and $y$, and for every $x$, equality is attained for some $y$*;

8. $B = GA^{-1}G$;

9. $G = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}$.

*Proof.* $1 \to 2$: By property 1,

$$B^{-1/2}AB^{-1/2} = \left(B^{-1/2}GB^{-1/2}\right)^2,$$

which implies property 2.

$2 \to 3$: Follows by choosing

$$U = A^{-1/2}B^{1/2}\left(B^{-1/2}AB^{-1/2}\right)^{1/2},$$

which clearly satisfies $UU^* = I$.

$3 \to 4$: Follows from

$$\begin{pmatrix} A & G \\ G & B \end{pmatrix} = \begin{pmatrix} A^{1/2} & 0 \\ 0 & B^{1/2} \end{pmatrix}\begin{pmatrix} I & U \\ U^* & I \end{pmatrix}\begin{pmatrix} A^{1/2} & 0 \\ 0 & B^{1/2} \end{pmatrix}$$

and the well-known fact

(F) for $P$ nonsingular of order $n$ and $Q$, $R$, and $S$ or order $n$,

$$\operatorname{rank}\begin{pmatrix} P & Q \\ R & S \end{pmatrix} = n$$

if and only if $S = RP^{-1}Q$.

$4 \to 1$: Follows from (F) again.

$4 \to 5$: Choose $x$ and define $y$ by $Ax = Gy$. By (F),

$$\begin{aligned} By &= GA^{-1}Gy \\ &= Gx. \end{aligned}$$

$5 \to 1$: Eliminating $y$ in property 5, we have $(GB^{-1}G - A)x = 0$ for all $x$, e.g. property 1.

$3 \to 6$: We have

$$\begin{aligned}|(Gx, y)|^2 &= |(Gy, x)|^2\\ &= |(UB^{1/2}y, A^{1/2}x)|^2\\ &\leqslant (B^{1/2}y, B^{1/2}y)(A^{1/2}x, A^{1/2}x)\\ &= (Ax, x)(By, y),\end{aligned}$$

and equality occurs with $y = B^{-1/2}U^*A^{1/2}x$.

$6 \to 7$: Immediate by $\operatorname{Re}(Gx, y) \leqslant |(Gx, y)|$ and the arithmetic–goemetric-mean inequality.

$7 \to 4$: Property 7 means that

$$(x^* y^*)\begin{pmatrix} A & G \\ G & B \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} \geqslant 0$$

together with the condition that for every $x$ there is some $y$ for which equality is attained. This, in its turn, is equivalent to the fact that the matrix in property 4 is positive semidefinite and has rank $n$.

$1 \to 8$: Clear.

$8 \to 9$ and $9 \to 3$: Analogous to the proof of the implications $1 \to 2 \to 3$. ■

Given matrices $A$ and $B$, observe that $G$ is the unique matrix satisfying any one of properties 1–9. It seems natural to write $G(A, B)$ for $G$ and to call it the *metric geometric mean* of the matrices $A$ and $B$.

The following properties of $G(A, B)$ are consequences of Theorem 2.1.

THEOREM 2.2. *Let $A$ and $B$ be positive definite matrices of order $n$. Then*

1. $G(A, B) = G(B, A)$;
2. *if $A$ and $B$ commute, then $G(A, B)$ commutes with each of $A$ and $B$ and*

$$G(A, B) = A^{1/2}B^{1/2};$$

3. *$G(A, B)$ is a nondecreasing function of each of its arguments, in the sense that*

$$G(A_1, B) \leqslant G(A_2, B) \qquad \textit{if} \quad A_1 \leqslant A_2,$$

*$\leqslant$ meaning the Loewner ordering, i.e. $P \leqslant Q$ if and only if $Q - P$ is positive semidefinite;*

4. *$G(A, B)$ is a continuous function of each of its arguments;*
5. $G(A^{-1}, B^{-1}) = [G(A, B)]^{-1}$;
6. *$G(XAX^*, XBX^*) = XG(A, B)X^*$ for any nonsingular matrix $X$;*
7. $\det G(A, B) = \sqrt{\det A \cdot \det B}$;
8. *for the $k$th compound matrix, $k = 2, \dots, n$,*

$$[G(A, B)]^{(k)} = G(A^{(k)}, B^{(k)});$$

9. $G(A, B) \leqslant \frac{1}{2}(A + B)$;
10. *if $H(A, B)$ is the harmonic mean of $A$ and $B$, i.e.*

$$H(A, B) = 2(A^{-1} + B^{-1})^{-1},$$

*then*

$$H(A, B) \leqslant G(A, B).$$

*In addition, if $A_1$, $B_1$ are positive definite matrices of the same order and $A_2$, $B_2$ positive definite matrices of the same order, then for the tensor products*

$$G(A_1 \otimes A_2, B_1 \otimes B_2) = G(A_1, B_1) \otimes G(A_2, B_2).$$

*Proof.* Properties 1–7 are immediate. To prove property 8, observe that the well-known property for multiplication

(C1) $(PQ)^{(k)} = P^{(k)}Q^{(k)}$

implies

(C2) $(P^{1/2})^{(k)} = (P^{(k)})^{1/2}$

for a positive definite matrix $P$.

Property 9 follows from

$$\tfrac{1}{2}(GB^{-1/2} - B^{1/2})(GB^{-1/2} - B^{1/2})^* \geqslant 0.$$

Property 10 is a consequence of properties 9 and 5.

The final assertion follows easily from multiplicative properties of tensor products. ∎

## 3. THE SPECTRAL GEOMETRIC MEAN

We intend to define now another geometric mean of two positive definite matrices $A$ and $B$. The definition is based on the following theorem, which also uses the notion of the metric geometric mean $G(A, B)$ defined above:

THEOREM 3.1. *Let $A$, $B$, and $F$ be positive definite matrices of order $n$. Then the following are equivalent:*

1. $G(A^{-1}, F) = G(F^{-1}, B)$;
2. $G(A^{-1}, F)G(B^{-1}, F) = I$;
3. *there exists a positive definite matrix $C$ such that both $F = CAC$ and $F = C^{-1}BC^{-1}$ hold;*
4. $F = G^{1/2}(A^{-1}, B)AG^{1/2}(A^{-1}, B)$;
5. $F=[B^{1/2}(B^{1/2}AB^{1/2})^{-1/2}B^{1/2}]^{1/2}A[B^{1/2}(B^{1/2}AB^{1/2})^{-1/2}B^{1/2}]^{1/2}$;
6. $F = [A^{1/2}(A^{1/2}BA^{1/2})^{-1/2}A^{1/2}]^{1/2}B[A^{1/2}(A^{1/2}BA^{1/2})^{-1/2}A^{1/2}]^{1/2}$;
7. $F = G^{1/2}(A, B^{-1})BG^{1/2}(A, B^{-1})$.

*Proof.* $1 \to 2$: Follows from property 5 of Theorem 2.2.

$2 \to 3$: Set $C = G(A^{-1}, F)$; then $C$ is positive definite and $F = CAC$ by property 9 of Theorem 2.1. By property 2 we have $C^{-1} = G(B^{-1}, F)$; hence, $F = C^{-1}BC^{-1}$.

$3 \to 4$: By property 3, $B = C^2AC^2$, so that

$$C^2 = G(A^{-1}, B)$$

and property 4 follows.

$4 \to 5$: An immediate consequence of property 2 of Theorem 2.1.

$5 \to 6$: By properties 2, 8 of Theorem 2.1, respectively, properties 5 and 6 read $F = G^{1/2}(A^{-1}, B)AG^{1/2}(A^{-1}, B)$ and $F = G^{1/2}(B^{-1}, A)BG^{1/2}(B^{-1}, A)$, which equals $G^{-1/2}(A^{-1}, B)BG^{-1/2}(A^{-1}, B)$. Since $G(A^{-1}, B)AG(A^{-1}, B) = B$, equality follows.

5 and $6 \to 1$: By property 8 of Theorem 2.1, the matrix $G(A^{-1}, F)$ is characterized as the unique positive definite matrix $M$ for which $F = MAM$. It follows from property 5 that

$$G(A^{-1}, F) = \left[B^{1/2}(B^{1/2}AB^{1/2})^{-1/2}B^{1/2}\right]^{1/2}.$$

Furthermore, property 2 of Theorem 2.1 yields

$$M = G(A^{-1}, F) = \left[G(A^{-1}, B)\right]^{1/2}.$$

In a similar manner, it follows from condition 6 that the unique matrix $N$ satisfying $B = NFN$ is

$$N = G(B, F^{-1}) = \left[A^{1/2}(A^{1/2}BA^{1/2})^{-1/2}A^{1/2}\right]^{-1/2};$$

furthermore, property 8 of Theorem 2.1 yields $N = G(A, B^{-1})^{-1/2}$, and property 5 of Theorem 2.2 gives $N = G(A^{-1}, B)^{1/2}$, so that $M = N$, in other words, property 1.

7 $\leftrightarrow$ 6: Immediate by property 9 of Theorem 2.1. ∎

The preceding theorem shows that the matrix $F$ is uniquely determined by the matrices $A$ and $B$. For reasons which will become clear in a moment, we shall call it the *spectral geometric mean* of the matrices $A$ and $B$ and denote it by $F(A, B)$. It will also be convenient to introduce the following terminological convention. We shall say that a matrix $Z$ is *positively similar* to a matrix $Y$ if there exists a positive definite matrix $P$ such that $Z = PYP^{-1}$.

THEOREM 3.2. *As a function of two positive definite matrices, the spectral geometric mean $F(\cdot, \cdot)$ has the following properties:*

1. *it is a positive definite matrix;*
2. $F(A, B) = F(B, A)$;
3. *for every unitary matrix $U$ of the same order.*

$$F(UAU^*, UBU^*) = UF(A, B)U^*;$$

4. $F(A^{-1}, B^{-1}) = F^{-1}(A, B)$;
5. *if $A$ and $B$ commute, then $F(A, B)$ commutes with both $A$ and $B$ and*

$$F(A, B) = A^{1/2}B^{1/2};$$

6. $F(A, B) = G^{1/2}(A^{-1}, B)AG^{1/2}(A^{-1}, B)$, *where $G(\cdot, \cdot)$ means the metric geometric mean from Theorem* 2.1;
7. $\det F(A, B) = \sqrt{\det A \cdot \det B}$;
8. $[F(A, B)]^2$ *is positively similar to $AB$; in particular, the eigenvalues of $F(A, B)$ are the positive square roots of the eigenvalues of $AB$ (and also $BA$) including multiplicities;*
9. *for the $k$th compound matrices, $k = 2, \ldots, n$,*

$$[F(A, B)]^{(k)} = F(A^{(k)}, B^{(k)});$$

10. *if* $A_1$, $B_1$ *are positive definite matrices of the same order and* $A_2$, $B_2$ *positive definite matrices of the same order, then for tensor products*

$$F(A_1 \otimes A_2, B_1 \otimes B_2) = F(A_1, B_1) \otimes F(A_2, B_2);$$

11. *if* $\lambda_{\max}$ $(\lambda_{\min})$ *denotes the maximum (minimum) eigenvalue, then*

$$\lambda_{\max}(F(A, B)) \geqslant \lambda_{\max}(G(A, B)),$$

$$\lambda_{\min}(F(A, B)) \leqslant \lambda_{\min}(G(A, B));$$

12. *if* $f_1 \geqslant f_2 \geqslant \cdots \geqslant f_n$ *are the eigenvalues of* $F(A, B)$ *and* $g_1 \geqslant g_2 \geqslant \cdots \geqslant g_n$ *the eigenvalues of* $G(A, B)$, *then*

$$\prod_{i=1}^{k} f_i \geqslant \prod_{i=1}^{k} g_i \qquad \text{for} \quad k = 1, \ldots, n-1,$$

$$\prod_{i=1}^{n} f_i = \prod_{i=1}^{n} g_i.$$

*Proof.* Properties 1–7 follow immediately from Theorems 2.2 and 3.1. Multiplication of the two equations in property 3 of Theorem 3.1 yields property 8.

Property 9 follows from property 5 of Theorem 3.1 and property 2 of Theorem 2.1, using the formulae (C1) and (C2) above.

A similar result for the tensor products yields property 10.

To prove property 11, define the matrix $Z = B^{-1/2}G(A, B)B^{1/2}$ so that $Z$ is similar to $G(A, B)$ and denote by $z$ a unit eigenvector of $Z$ corresponding to $\lambda_{\max}(G(A, B))$. Then

$$\begin{aligned} \lambda^2_{\max}(G(A, B)) &= (Zz, Zz) \\ &= (z, Z^*Zz) \\ &= (z, B^{1/2}AB^{1/2}z) \end{aligned}$$

by property 1 of Theorem 2.1. Since $B^{1/2}AB^{1/2}$ is similar to $F^2(A, B)$ by property 8,

$$\lambda^2_{\max}(G(A, B)) \leqslant \lambda^2_{\max}(F(A, B)).$$

The second of the inequalities follows by applying the inequality just proved to $A^{-1}$ and $B^{-1}$ using property 5 of Theorem 2.2 and property 4 of the present theorem.

Finally, property 12 is an immediate consequence of properties 10 and 11, since $\prod_1^k f_i$ etc. is the maximum eigenvalue of $F(A^{(k)}, B^{(k)})$ etc. ■

REMARK 3.3. The conditions in property 12 are identical with the well-known necessary and sufficient conditions of H. Weyl [6] and A. Horn [5] for the existence of an $n$-by-$n$ complex matrix with singular values $f_i$ and such that its eigenvalues $\lambda_i$ satisfy $|\lambda_i| = g_i$.

REMARK 3.4. One of the most important properties of the function $F(A,B)$ is the fact that its square is positively similar to $AB$ (see property 8 of the preceding theorem). This property does not characterize $F(\cdot,\cdot)$, however.

To show that, set $F_1 = (A^{1/2}BA^{1/2})^{1/2}$, $F_2 = (B^{1/2}AB^{1/2})^{1/2}$, so that both $F_1$ and $F_2$ are positive definite. The identities

$$F_1^2 = A^{-1/2}(AB)A^{1/2},$$

$$F_2^2 = B^{1/2}(AB)B^{-1/2}$$

show that both $F_1^2$ and $F_2^2$ are positively similar to $AB$. To see that $F_1$ and $F_2$ are not equal in general, it suffices to show that $F_1 = F_2$ if and only if $A$ and $B$ commute. Indeed, suppose $F_1 = F_2$. We have then $A^{1/2}BA^{1/2} = B^{1/2}AB^{1/2}$. Setting $R = A^{1/2}B^{1/2}$, this identity appears in the form $RR^* = R^*R$, so that $R$ is normal. The spectrum of $R$ being positive, we conclude that $R$ is Hermitian, $R = R^*$, and this implies $AB = BA$. The converse is immediate.

## 4. COMPARISON THEOREMS

In this section, we shall first compare the geometric means $F(A, B)$ and $G(A, B)$ with $A$ and $B$ in the case that $A \leqslant B$. In the proof, the following lemma will be of importance.

LEMMA 4.1. *Let $X$ be a positive definite matrix. Then the following assertions are equivalent*:

1. $X \leqslant I$;
2. $X^2 \leqslant I$;
3. $X^2 \leqslant X$.

*Proof.* Clear. ■

THEOREM 4.2. *Suppose $A$ and $B$ are positive definite matrices of the same order. Then the following assertions are equivalent*:

1. $B \leqslant A$;
2. $G(A, B) \leqslant A$;
3. $B \leqslant G(A, B)$.

*Proof.* If $B \leqslant A$ then $A^{-1/2}BA^{-1/2} \leqslant I$; hence, by Lemma 4.1, $(A^{-1/2}BA^{-1/2})^{1/2} \leqslant I$, so that

$$G(A, B) = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2} \leqslant A.$$

If $G(A, B) \leqslant A$ then $(A^{-1/2}BA^{-1/2})^{1/2} \leqslant I$, so that $A^{-1/2}BA^{-1/2} \leqslant I$ by Lemma 4.1; hence,

$$B = A^{1/2}(A^{-1/2}BA^{-1/2})A^{1/2} \leqslant A,$$

and this implies $B = G(B, B) \leqslant G(A, B)$ by condition 3 of Theorem 2.2.

If $B \leqslant G(A, B)$ then

$$A^{-1/2}BA^{-1/2} \leqslant A^{-1/2}G(A, B)A^{-1/2} = (A^{-1/2}BA^{-1/2})^{1/2}.$$

By Lemma 4.1, it follows that $(A^{-1/2}BA^{-1/2})^{1/2} \leqslant I$, so that $G(A, B) \leqslant A$ and, consequently, $B \leqslant G(A, B) \leqslant A$. ■

In the following theorem, we shall describe the behavior of the function $F(A, B)$.

THEOREM 4.3. *Let $A$, $B$ be positive definite matrices of the same order $n$. Then the properties*

$$F(A, B) \leqslant A \quad \textit{and} \quad B \leqslant F(A, B)$$

*are equivalent.*

*On the other hand, for $n > 1$, the inequality $B \leqslant A$ does not imply those properties.*

*Proof.* Suppose that $F(A, B) \leqslant A$. Set $H = G(A^{-1}, B)$, so that $B = HAH$ and $F(A, B) = H^{1/2}AH^{1/2}$. We have then

$$B = HAH = H^{1/2}F(A, B)H^{1/2} \leqslant H^{1/2}AH^{1/2} = F(A, B).$$

If $B \leqslant F(A, B)$ then $B \leqslant H^{1/2}AH^{1/2}$; hence, $F(A, B) = H^{-1/2}BH^{-1/2} \leqslant A$.

The last assertion follows from the example

$$A = \begin{pmatrix} \frac{7}{108} & \frac{1}{36} \\ \frac{1}{36} & \frac{1}{81} \end{pmatrix}, \qquad B = \begin{pmatrix} \frac{28}{27} & 1 \\ 1 & 1 \end{pmatrix},$$

for which

$$F(A, B) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{3} \end{pmatrix}.$$

It is easily checked that $B > A$ but $B \not\geqslant F(A, B)$. ■

REMARK 4.4. The above example shows also that in general, $F(A, B) \not\leqslant \frac{1}{2}(A + B)$.

Though $F(A, B)$ lacks the betweenness property, it enjoys two other properties which, in fact, attracted the authors to this topic. The symbol $\sigma(Z)$ means the spectrum of $Z$.

THEOREM 4.5. *Suppose $A$ and $B$ are positive definite. Then the following assertions are equivalent*:

1. $B^{-1} \leqslant A$;
2. $A^{-1} \leqslant B$;
3. $\sigma(AB) \geqslant 1$;
4. $\sigma(BA) \geqslant 1$;
5. $A^{1/2}BA^{1/2} \geqslant I$;
6. $B^{1/2}AB^{1/2} \geqslant I$;
7. $F(A, B) \geqslant I$.

*Proof.* We prove the following cycle of implications:

$$1 \to 3 \to 5 \to 2 \to 4 \to 6 \to 1$$

and the equivalence $3 \leftrightarrow 7$.

Assume $B^{-1} \leqslant A$, and suppose $ABx = \lambda x$ for some $x \neq 0$. Then

$$\lambda(x, Bx) = (ABx, Bx) \geqslant (B^{-1}Bx, Bx) = (x, Bx) > 0;$$

hence, $\lambda \geqslant 1$ which proves assertion 3. If $\sigma(AB) \geqslant 1$ then $\sigma(A^{1/2}BA^{1/2}) = \sigma(A^{-1/2}(AB)A^{1/2}) = \sigma(AB) \geqslant 1$. Since $A^{1/2}BA^{1/2} \geqslant 0$, it follows that $A^{1/2}BA^{1/2} \geqslant I$. We have thus proved the implications $1 \to 3 \to 5$. The same argument may be used to prove the implications $2 \to 4 \to 6$. We shall complete the proof of the cycle by proving the implications $5 \to 2$ and $6 \to 1$.

If $A^{1/2}BA^{1/2} \geqslant I$ then

$$B - A^{-1} = A^{-1/2}(A^{1/2}BA^{1/2} - I)A^{-1/2} \geqslant 0.$$

In this manner, assertion 5 implies assertion 2, and, by symmetry, assertion 6 implies assertion 1. The equivalence of assertions 3 and 7 follows from property 8 of Theorem 3.2. ■

Before proving the second theorem, we state the following lemma.

LEMMA 4.6. *Let $F$ be a positive matrix. Then the following are equivalent:*

1. $F \geqslant I$;
2. *there exists a matrix $X$ such that $\begin{pmatrix} F & X \\ X^* & F \end{pmatrix}$ is positive definite and*

$$\begin{pmatrix} F & X \\ X^* & F \end{pmatrix}^{-1} = \begin{pmatrix} F & Y \\ Y^* & F \end{pmatrix}. \tag{1}$$

*for some $Y$.*

*Proof.* $1 \to 2$: By Lemma 4.1, the matrix $F^2 \geqslant I$; set $X = \sqrt{F^2 - I}$. If $Y$ in (1) is chosen as $-\sqrt{F^2 - I}$, then (1) will be fulfilled.

$2 \to 1$: Let (1) be fulfilled for some $X$ and $Y$. Then, along with other relations,

$$F^2 + XY^* = I,$$
$$X^*F + FY^* = 0.$$

It follows that

$$F^2 - XF^{-1}X^*F = I,$$

which implies that $XF^{-1}X^*F$ is Hermitian, so that $F$ (and $F^{1/2}$) commutes with $XF^{-1}X^*$. Therefore

$$F^2 - I = (F^{1/2}XF^{-1/2})(F^{1/2}XF^{-1/2})^*.$$

The right-hand side is positive, which implies assertion 1. ■

THEOREM 4.7. *Let $A$ and $B$ be positive definite matrices of the same order. Then $F(A, B) \geqslant I$ if and only if the following condition is satisfied:*

8. *there exist matrices $X$ and $Y$ such that*

$$T = \begin{pmatrix} A & X \\ X^* & B \end{pmatrix}$$

*is positive definite and*

$$T^{-1} = \begin{pmatrix} B & Y \\ Y^* & A \end{pmatrix}.$$

REMARK 4.8. Condition 8 completes the set of equivalent conditions stated in Theorem 4.2.

*Proof.* Let condition 8 be fulfilled for some $X$. By property 3 of Theorem 3.1, there exists a positive definite matrix $C$ such that $F(A, B) = CAC$ as well as $F(A, B) = C^{-1}BC^{-1}$.

Define the block-diagonal matrix $Q = \mathrm{diag}(C, C^{-1})$. The matrix $QTQ$ has the form mentioned in Lemma 4.6 and satisfies (1). By the lemma, $F(A, B) \geqslant I$. The converse is also true, since if $F(A, B) \geqslant I$ and if $Z$ is the matrix on the left-hand side of (1), then the matrix $Q^{-1}ZQ^{-1}$ satisfies condition 8. ■

## 5. CONCLUDING REMARKS

It is easily seen that for $n \geqslant 2$ the geometric means $G(A, B)$ and $F(A, B)$ are generally distinct. From possible strict inequalities in property 11 of Theorem 3.2 it follows that $G(A, B)$ and $F(A, B)$ are in general not comparable in the Loewner ordering. The two means are, however, equal if the matrices $A$ and $B$ commute, and one may ask if this is the only case when $G(A, B)$ and $F(A, B)$ coincide. We shall be able to give an affirmative answer in Theorem 5.2. In the proof, we shall need a lemma.

LEMMA 5.1. *Let $P$ and $Q$ be positive definite matrices, and let*

$$PQPQ^{-1} = QPQ^{-1}P. \tag{2}$$

*Then $PQ = QP$.*

*Proof.* Multiplying (2) by $Q^{-1/2}$ from the left and by $Q^{1/2}$ from the right, we obtain $RR^* = R^*R$, where $R$ is the matrix $Q^{-1/2}PQ^{1/2}$. It follows that $R$ is normal and thus Hermitian, since its eigenvalues are real.

This means

$$Q^{-1/2}PQ^{1/2} = Q^{1/2}PQ^{-1/2},$$

i.e. $PQ = QP$. ∎

THEOREM 5.2. *For two positive definite matrices $A$ and $B$ of the same order, the metric and spectral geometric means $G(A, B)$ and $F(A, B)$ coincide if and only if $A$ and $B$ commute.*

*Proof.* As we already observed, just the "only if" part has to be proved. Thus suppose that $F(A, B) = G(A, B) = F$. It follows that

$$A = FB^{-1}F. \tag{3}$$

Set

$$H = G^{1/2}(A, B^{-1}),$$

so that

$$F = H^{-1}AH^{-1} = HBH.$$

It follows that $A = HFH$ and $B^{-1} = HF^{-1}H$. Substituting these expressions in (3), we obtain

$$HFH = FHF^{-1}HF;$$

hence,

$$HFHF^{-1} = FHF^{-1}H.$$

By Lemma 5.1, $HF = FH$, and since

$$AB = HF^2H^{-1},$$

$$BA = H^{-1}F^2H,$$

$A$ and $B$ commute. ∎

We intend to investigate more thoroughly the relationship between the functions $F(A, B)$ and $G(A, B)$ corresponding to the same pair of matrices $A$ and $B$. We shall first state a lemma.

LEMMA 5.3. *If $A$ is a complex matrix, then*

$$(AA^*)^{1/2}A = A(A^*A)^{1/2}.$$

*Proof.* The intertwining relation

$$AA^* \cdot A = A \cdot A^*A$$

implies

$$p(AA^*)A = Ap(A^*A)$$

for every polynomial $p$. Using the fact that both matrices $AA^*$ and $A^*A$ have the same characteristic polynomial as well as the fact that their positive square roots are limits of the same polynomials, the result follows. ∎

COROLLARY 5.4. *If $A$ is a nonsingular complex matrix, then*

$$(AA^*)^{1/2} = A(A^*A)^{-1/2}A^*.$$

*Proof.* By Lemma 5.3,

$$\begin{aligned}(AA^*)^{1/2}A^{*-1}(A^*A)^{1/2}A^{-1} &= A(A^*A)^{1/2}A^{-1}A^{*-1}(A^*A)^{1/2}A^{-1}\\ &= A(A^*A)^{1/2}(A^*A)^{-1}(A^*A)^{1/2}A^{-1}\\ &= I.\end{aligned}$$ ∎

THEOREM 5.5. *Suppose $F$ and $G$ are positive definite matrices of the same order. Then the following assertions are equivalent:*

1. *there exists a pair of positive definite matrices $A$ and $B$ such that $F = F(A, B)$ and $G = G(A, B)$;*
2. *there exists a positive definite matrix $C$ such that*

$$F = (CGC^{-1})^* F^{-1}(CGC^{-1});$$

3. *there exists a positive definite matrix $C$ such that*

$$G = C^{-1}F^{1/2}(F^{-1/2}C^2FC^2F^{-1/2})^{1/2}F^{1/2}C^{-1};$$

4. *there exist two invertible matrices $P$ and $Q$ such that $F^{1/2}Q$ is positive definite and*

$$F = Q^{*-1}P,$$

$$G = Q^{-1}(QPP^*Q^*)^{1/2}Q^{*-1};$$

5. *$G$ is positively similar to $F^{1/2}UF^{1/2}$ suitable unitary $U$.*

*Proof*. Suppose first that $F = F(A, B)$ and $G = G(A, B)$ for some positive definite matrices $A$ and $B$. Then there exists a positive definite matrix $C$ such that $F = CAC$ as well as $F = C^{-1}BC^{-1}$ are satisfied. It follows that $A = C^{-1}FC^{-1}$ and $B = CFC$; hence,

$$CFC = B = GA^{-1}G = G(CF^{-1}C)G,$$

which implies assertion 2.

$2 \to 3$: The identity

$$CFC = G(CF^{-1}C)G$$

implies

$$C^2FC^2 = CGCF^{-1}CGC$$

and

$$\begin{aligned} F^{-1/2}C^2FC^2F^{-1/2} &= F^{-1/2}CGCF^{-1}CGCF^{-1/2} \\ &= (F^{-1/2}CGCF^{-1/2})^2. \end{aligned}$$

It follows that

$$F^{-1/2}CGCF^{-1/2} = \left(F^{-1/2}C^2FC^2F^{-1/2}\right)^{1/2}$$

and this implies assertion 3.

$3 \to 4$: Set $P = CF^{1/2}$ and $Q = F^{-1/2}C$. Then $F^{1/2}Q = C$ is positive definite and $F = P^*Q^{-1}$. At the same time,

$$G = Q^{-1}(QPP^*Q^*)^{1/2}Q^{*-1}.$$

$4 \to 5$: Set $A = QP$, which also means $A = QQ^*F$. The matrix $U$ defined by $U = A^{-1}(AA^*)^{1/2}$ is unitary. Since

$$\begin{aligned} F^{1/2}A^{-1} &= F^{-1/2}Q^{*-1}Q^{-1} \\ &= \left(Q^*F^{1/2}\right)^{-1}Q^{-1}, \end{aligned}$$

we obtain

$$\begin{aligned} F^{1/2}UF^{1/2} &= F^{1/2}A^{-1}(AA^*)^{1/2}F^{1/2} \\ &= \left(Q^*F^{1/2}\right)^{-1}Q^{-1}(QPP^*Q^*)^{1/2}Q^{*-1}(Q^*F^{1/2}) \\ &= \left(Q^*F^{1/2}\right)^{-1}G(Q^*F^{1/2}), \end{aligned}$$

which proves assertion 5.

$5 \to 2$: Suppose $G = MF^{1/2}UF^{1/2}M^{-1}$ for some positive definite $M$ and some unitary $U$. We have then

$$\begin{aligned} I &= U^*U \\ &= F^{-1/2}MGM^{-1}F^{-1/2}F^{-1/2}M^{-1}GMF^{-1/2}, \end{aligned}$$

whence

$$F = MGM^{-1}F^{-1}M^{-1}GM,$$

and this is assertion 2.

The proof will be complete if we prove the implication $2 \to 1$. Thus, let

$$F = (CGC^{-1})^{*} F^{-1}(CGC^{-1}).$$

Set $A = C^{-1}FC^{-1}$, $B = CFC$. Then

$$GA^{-1}G = GCF^{-1}CG,$$

which can be written as

$$C \cdot C^{-1}GCF^{-1}CGC^{-1}C,$$

i.e. $CFC$, which equals $B$. Consequently, $G = G(A, B)$ by property 8 of Theorem 2.1.

At the same time,

$$F = CAC = C^{-1}BC^{-1},$$

so that $F = F(A, B)$ by property 3 of Theorem 3.1. ∎

REMARK 5.6. Under the hypotheses of assertion 4 it is possible to show that

$$Q^{-1}(QPP^{*}Q^{*})^{1/2}Q^{*-1} = P(P^{-1}Q^{-1}Q^{*-1}P^{*-1})^{1/2}P^{*}.$$

Indeed, using Corollary 5.4 for $A = QP$, this follows immediately.

In a similar manner, setting $P = CF^{1/2}$ and $Q = F^{-1/2}C$, we obtain another identity for arbitrary positive definite matrices $C$ and $F$:

$$C^{-1}F^{1/2}(F^{-1/2}C^{2}FC^{2}F^{-1/2})^{1/2}F^{1/2}C^{-1}$$
$$= CF^{1/2}(F^{-1/2}C^{-2}FC^{-2}F^{-1/2})^{1/2}F^{1/2}C.$$

Let us now ask whether the notions $G(A, B)$ and $F(A, B)$ of metric and spectral geometric mean can be generalized to the case that one or both matrices $A$ and $B$ are singular and positive without losing good properties.

The situation with $G(A, B)$ is then the following. It can be well defined if $A$ and $B$ have the same range. In that case, $G(A, B)$ is uniquely defined (and has the same range) by the condition that it is the positive matrix $G$ for which

$$\operatorname{rank}\begin{pmatrix} A & G \\ G & B \end{pmatrix} = \operatorname{rank} A \tag{4}$$

holds.

It is then easily seen that the following summarizing theorem holds [the symbol $P^+$ means as usual the Moore-Penrose inverse of $P$ (cf. [2]), and observe that for positive matrices, $(P^{1/2})^+ = (P^+)^{1/2}$].

THEOREM 5.7. *Let $A$ and $B$ be positive matrices with the same range, and let $P$ be the matrix of the orthogonal projection on that range. Then the metric geometric mean $G(A, B)$ of $A$ and $B$ defined by* (4) *has the following properties*:

1. $G(A, B) = B^{1/2}(B^{1/2\,+}AB^{1/2\,+})^{1/2}B^{1/2}$;
2. $A = G(A, B)B^+G(A, B)$;
3. *for the matrix* $U = A^{1/2\,+}B^{1/2}(B^{1/2\,+}AB^{1/2\,+})^{1/2}$ *which satisfies* $UU^* = P$,

$$G(A, B) = A^{1/2}UB^{1/2};$$

4. $G(A^+, B^+) = G^+(A, B)$;
5. $G(A, B) \leqslant \frac{1}{2}(A + B)$;
6. *for every matrix $X$ for which $XA$ exists*,

$$G(XAX^*, XBX^*) = XG(A, B)X^*.$$

The situation with the spectral geometric mean is different. If we take as definition of $F(A, B)$, which seems to be most appropriate, property 3 in Theorem 3.1, then the rank of $F$ has to be the same as the rank of both $A$ and $B$, and even the same as the rank of $AB$.

Thus the condition

$$\text{rank } A = \text{rank } B = \text{rank } AB$$

is clearly necessary for the existence of a positive definite $C$ for which $CAC = C^{-1}BC^{-1}$. It is possible to show that it is also sufficient; uniqueness of $C$, however, is not guaranteed without additional assumptions. Thus, there are more than one candidate for the definition of $F(A, B)$. This situation is illustrated by the following example.

EXAMPLE 5.8. Let

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

For any $k > 1$, the matrix

$$C(k) = \frac{1}{\sqrt{k^2+1}} \begin{pmatrix} k & 1 \\ 1 & k^2 - k + 1 \end{pmatrix}$$

is positive definite and

$$[C(k)]^{-1} = \frac{1}{(k-1)\sqrt{k^2+1}} \begin{pmatrix} k^2 - k + 1 & -1 \\ -1 & k \end{pmatrix}.$$

It is easily checked that then $C(k)AC(k)$ equals $C(k)^{-1}BC(k)^{-1}$ and this matrix $F(k)$ is

$$F(k) = \frac{1}{k^2+1} \begin{pmatrix} k^2 & k \\ k & 1 \end{pmatrix}.$$

Each of these matrices $F(k)$ can thus be considered as the spectral geometric mean of $A$ and $B$.

Observe also that for sufficiently large $k$, $F(k)$ does not satisfy

$$F(k) \leqslant \tfrac{1}{2}(A+B).$$

On the other hand, each $F(k)$ has the eigenvalues 1 and 0, which are the square roots of the eigenvalues of $AB$.

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*Received 2 February 1995; final manuscript accepted 5 June 1995*